How close are two grain boundaries?

(In the five-dimensional macroscopic crystallographic space.)

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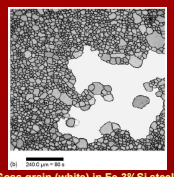
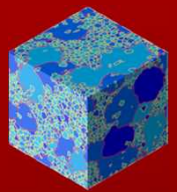
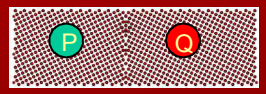
A distance is needed to interpolate into a table of grain boundary properties



Goss grain (white) in Fe-3%Si steel
A. L. Etter *et al., Scripta Mater.* 47 725 (2002)



simulation captures abnormal growth phenomenology
(Courtesy of E.A. Holm)



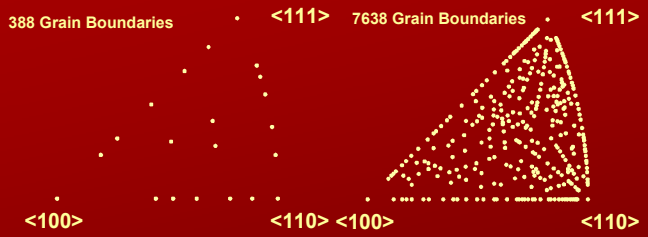
- For mesoscale simulations we need to assign properties to an any boundary.
- To look up an arbitrary boundary in table, we need to find the most similar boundary in the table.
- The natural assumption is that boundaries close in crystallographic space will have similar properties.
- This assumption needs to be tested.

Previous 5d distances

- A. Morawiec has proposed a specific distance based on misorientation and boundary normals: Proceedings of the Third International Conference on Grain Growth, TMS, Warrendale, 1998, p. 509; Acta. Mat., 48 (2000) 3525.
- J.W. Cahn & J.E. Taylor have given a general discussion of distances based on misorientation and boundary normals:
  J. Mater. Sci., 41 (2006) 7669.
- These distances require an arbitrary choice of how much to weight to give to differences in misorientation, and how much to differences in boundary normal.

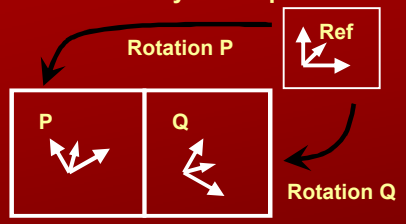
Need distance to fill in holes in the table.

Disorientation axes (smallest angle) in a table of boundaries:



Add boundaries from larger set where there are holes, not all of them.

Describe a boundary in 5d space

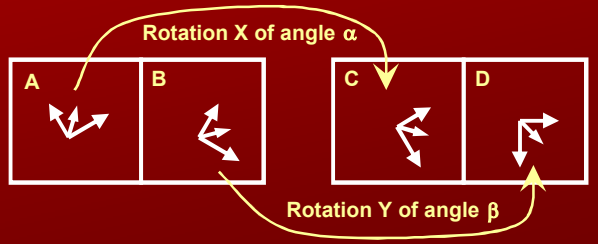


(P,Q) describes boundary, but we have to allow for fcc symmetries and rotations about boundary normal.

$$(\mathbf{P},\mathbf{Q}) \equiv (\mathbf{UPT}_1, \mathbf{UQT}_2)$$

Where T_1 and T_2 are rotations that are fcc symmetries, and U is a rotation about the boundary normal.

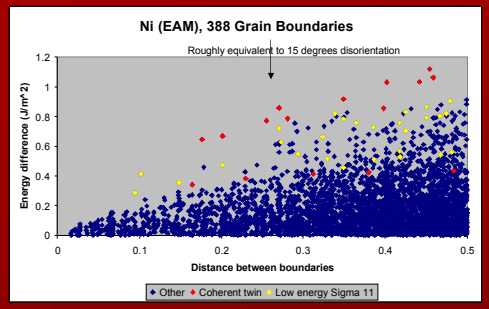
Distance between two boundaries



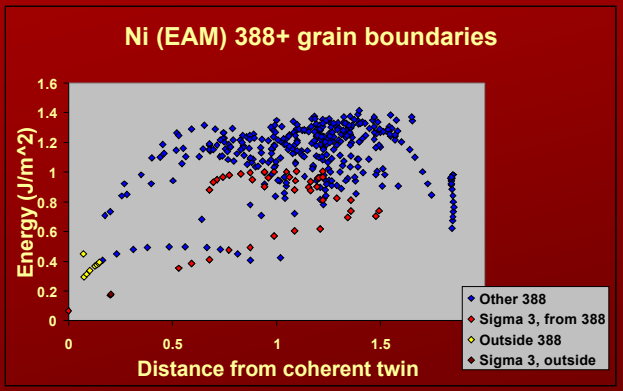
$$d(\mathbf{AB},\mathbf{CD}) = 2\sqrt{2}\sqrt{\sin^2(\alpha/2)+\sin^2(\beta/2)} \cong \sqrt{2}\sqrt{\alpha^2+\beta^2}$$

d is minimized over all equivalent representations of boundaries AB and CD

Boundaries which are close have similar energies.



Ni (EAM) 388+ grain boundaries



Conclusions

- A distance is needed to access a table of grain boundary properties for an arbitrary boundary.
- Distance is needed to choose boundaries to fill in holes in the table.
- For the distance shown here, nearby boundaries have similar energy.
- Distance can also be used to examine, e.g., the existence of energy cusps.

Examples: D.L. Olmsted, S. Foiles, E.A Holm, in preparation.